

Stabilized FE Simulations of Transport/Reaction Systems: Algorithms and Applications

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In this talk I will discuss a stabilized finite element formulation for reacting flow applications based on the Galerkin Least Squares (GLS) method. This formulation is used to simulate reacting flow applications for incompressible, variable density and low Mach number compressible fluid flow, heat transfer and mass transfer with non-equilibrium chemical reactions. These systems are characterized by highly nonlinear, multiple time and length scale physics governed by coupled systems of PDEs. The numerical solution of these systems can be very challenging.

This presentation will overview a number of the important solution methods that we have applied in the computational simulation of transport/reaction systems. These include, fully-implicit time integration techniques using parallel nonlinear and linear solution methods based on Newton-Krylov iterative techniques. The nonlinear solution method is based on an inexact Newton method. This local method is globalized using residual backtracking. The resulting large sparse linear systems are solved by the application of parallel preconditioned Krylov methods using additive Schwarz domain decomposition (DD) preconditioners with subdomain ILU solvers. Preliminary results of an alternate multi-level strategy employing 2 level DD as well as block approximate factorizations with algebraic multigrid methods will also be presented.

To demonstrate the capability of these methods I will present simulation results for some representative low heat release and high heat release transport / reaction simulations. In this context we briefly discuss robustness, efficiency and scaling of the solution methods.

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